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Title: A Logic Model for Cook-off Phenomenology in High Explosives

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Abstract

Logic models are valuable tools in the development of predictive models for complex physical processes. The use of deductive logic in the form of a possibility tree makes it straightforward to develop a comprehensive set of unique, alternative paths that describe the system. We demonstrate the power of this approach for the complex process of cook-off of high explosives (HE). The possibility tree describes the causal paths from heating HE to the alternative end states. One of these end states is a violent reaction. Conversion of the tree to the equivalent digraph yields a valuable visualization tool for examining the relationships between sub-processes and provides a sound framework for the development of analytical models.

Introduction

High explosives (HE) can pose a serious potential hazard for the personnel who manufacture, transport, store and use them. The danger arises from the fact that under certain circumstances, relatively small mechanical or thermal stimuli can lead to a very rapid energy release, referred to as a high explosive violent reaction (HEVR), a class of reactions ranging up to a detonation. The likelihood of an HEVR is known to depend upon a number of factors including the type of explosive, its physical configuration and the nature and strength of the stimulus. In general these dependencies are known at best only approximately and the capability to predict the likelihood of an HEVR with reasonable confidence is only possible for a relatively small set of specific conditions.

The HEVR hazard is well known and many historical events testify to the tremendous damage that an HEVR can cause. This is particularly true for conventional high explosives (CHE) used in military applications. The large number of munitions, the necessity to use and store them in large quantities and the frequency of significant stimuli in training, handling and combat environments all combine to increase the risk associated with an HEVR. There are far fewer nuclear weapons than conventional munitions and their stockpile to target sequences are quite different. However the potential consequences of an HEVR in a nuclear weapon mean that understanding the conditions leading to an HEVR are important for these weapons as well. One major branch of HE research at Los Alamos National Laboratory is the study of HEVR in the plastic-bonded explosives (PBXs) used in U.S. nuclear weapons. Similar PBXs are used in certain high performance military munitions. A PBX of particular interest is PBX 9501 (95% HMX, 2.5% Estane, 2.5% plasticizer), a CHE.

In this paper we consider the phenomenology of cook-off in PBXs. Although the ultimate goal of our research is the development of predictive models for HEVR in cook-off environments, the first objective in this project is different. We are attempting to build a logic model for cook-off that describes possible phenomenological paths to HEVR in a thermal environment. Because the knowledge of the physical and chemical processes is incomplete and therefore uncertain, the model is designed to facilitate the discovery and representation of *alternative* paths to HEVR. The capability of a logic model to explicate these alternatives provides a number of useful features that will be made clear below. The paper considers specifically cook-off in PBX 9501. However the logic model and the results obtained from it will be generally useful for other PBXs, including insensitive HEs (IHE). We begin with a short review of cook-off phenomenology. The intention here is to introduce the phenomenological concepts that will appear in the logic model. In the next Section we introduce the basic concepts of logic models and place them in the context of a decision model. These preliminaries lead to the presentation of the cook-off model and an extended description of its structure. This is followed by a discussion of some of the results obtained from the work on the model to date and their implications for cook-off research.

Cook-off Phenomenology in Plastic-bonded Conventional Explosives

PBX 9501 recently has been the subject of a number of experiments at Los Alamos and elsewhere (ref. 1) aimed at understanding its response in slow heating environments. This attention is the result of the discovery that slow heating can lead to extremely violent reactions, approaching, and possibly reaching a detonation. Previously it was believed that PBX 9501 would not exhibit HEVR behavior in slow heat environments. Experiments have revealed that processes leading from a pristine explosive to detonation pass through a continuum of states, often involving complex interactions among physical, chemical and mechanical phenomena. The nature and number of important processes change with time as the cook-off progresses. The time scales of the interactions range from hours for the initial endothermic decomposition processes down to the microsecond scale characteristic of a detonation. The characteristic length scales vary similarly. These features of cook-off phenomenology make it difficult to diagnose and interpret experiments and to develop predictive models.

Numerical simulations are problematic as well because neither the basic physical processes nor their interactions with each other or the boundary conditions are well understood. The character of those processes that are known is such that algorithm design is difficult. For example, initially the primary problem is to predict the slow flow of thermal energy into the system, the endothermic chemical response of the HE and the redistribution of materials with widely varying properties. Later phases of the process progressively involve evolving damage to the HE microstructure, increasing exothermicity and faster response times. The effects of confinement must also be appropriately accounted for throughout this entire sequence.

The phenomenology of cook-off in PBX 9501 leading to detonation roughly follows the sequence: Heat inflow from the heated boundaries leads to a highly endothermic solid phase transition of the HMX (onset approximately 150 C) causing a significant volume expansion and potential mechanical damage depending upon the available ullage and the strength of the system confinement. Continued heating induces chemical reactions that are initially mildly endothermic, then mildly exothermic and finally highly exothermic. The highest temperatures and thus the early exothermicity occurs nearest the heated boundaries. At some point the direction of heat flow reverses and the region of highest temperatures moves inward to the interior of the HE. This process is essential to obtaining a violent outcome – faster heating produces ignition near the surface of the HE and leads to simple burning or disassembly of the charge. Eventually continued heating leads to runaway exothermic reactions – a thermal explosion. The thermal explosion can lead to immediate system disassembly or signal the initiation of burning. It is believed that the flow of product gases through the previously damaged microstructure can lead to preheating of adjacent material and therefore acceleration of the burning process – that is, convective burning. This burning in turn can further accelerate by causing additional flow in the damaged solid ahead of the burn front. This flow can lead to the appearance of a shock wave. The shock induces further acceleration of the exothermic decomposition leading to a deflagration to detonation transition (DDT). DDT is a poorly understood process, especially as it applies to PBXs. As suggested by this short description, there are branch points in this sequence that lead to outcomes other than detonation. There are discrepancies between experiments and models such as Frank-Kamenetskii thermal explosion theory (ref. 2). There are even more theories dealing with the acceleration of burning, primarily because experiments with PBXs are few in number and the paucity of suitable measurements. Although DDT has been studied for many years, there are still alternative, competing theories. Under these circumstances, the use of logic models offers the potential to clarify the phenomenology under study by organizing the phenomenology into a coherent process and to identify alternative paths along which it can evolve.

Developing A Model in LED

Logic models have many applications in science and engineering. One of the most important is decision analysis. One may briefly summarize the steps in a decision process as follows:

1. Determine the possible alternatives
2. Define a preference metric to choose among the alternatives
3. Develop an inferential model to infer the metric for each alternative
4. Evaluate the metric for the alternatives and rank order them
5. Express the uncertainty associated with the rank ordering

Our research has lead to an approach to the decision process called Logic-evolved Decision analysis (LED). Underlying LED is the use of linked logic models. We refer to these models as the possibility and inference trees. The possibility tree provides the framework for using deduction to obtain the comprehensive set of alternatives needed to make a decision, Step 1 in the process outlined above. The inference tree provides a similar structure for Step 3. The emphasis in this paper is on a possibility tree describing cook-off phenomenology that allows us to deduce the alternative paths to HEVR mentioned earlier. We note in passing that potential decisions for which this possibility tree provides alternatives include the choice of mathematical models for cook-off, design of experiments and the estimate of risk under accident conditions.

Structure of a Possibility Tree: A possibility tree is classified as either causal or resultant. In a causal tree one begins with the final state and deduces the intervening processes, events and states, arriving eventually at the initial states. A fault tree used to represent the possible failure modes of an engineered system is one familiar form of causal possibility tree. In a resultant tree the deductive sequence is reversed. The choice of which type of possibility tree to construct is problem-dependent and is influenced additionally by the available knowledge and the preferences of the analyst. The cook-off possibility tree presented here is of the resultant type.

Figure 1 shows a simple resultant possibility tree that illustrates many of the properties that these logic models possess. This tree was constructed using LED TREE, part of the software package LED TOOLS under development at Los Alamos (ref. 3). The top node in the tree is the initial state. We consider this node (*Initial Cycle*) to be the start of a physical process that is cyclic in nature. This is indicated by the icon to its left that represents the logic associated with a cycle. By convention the last input (*Exit from the initial cycle to*) defines how to exit the cycle. The first exit is always the return to the start of the cycle (*The start of the initial cycle*). The inputs above the exit describe a sequence of process associated with the cycle. The first and third inputs (*First process* *step, Third process step*) appear with the terminal icon, indicating that no more deduction is needed. The second input (*Possible second process steps*) shows the exclusive OR icon. In this instance two mutually exclusive ways in which to realize the second process have been deduced. This is the first indication of the presence of alternative paths. Returning now to the exit from the cycle gate, we see that it is also defined by exclusive OR logic. In addition to the previously mentioned return to the beginning of the cycle, we deduce that it also possible to exit to two distinct final states (*End State A, End State B*). In the language of LED TREE these are denoted as replicants, indicating that they may appear more than once in the tree. Replicants can be far more complex than a simple terminal node. The last exit from the first cycle is another cycle (*The start of second cycle*), with exactly the same logical structure as the first. We observe that it exits to the same end states as in the first cycle as well as an additional one (*End State C*). The ability to link together cycle gates and to use replicants as inputs to different logic gates makes it possible to create very complex and detailed logical sequences.

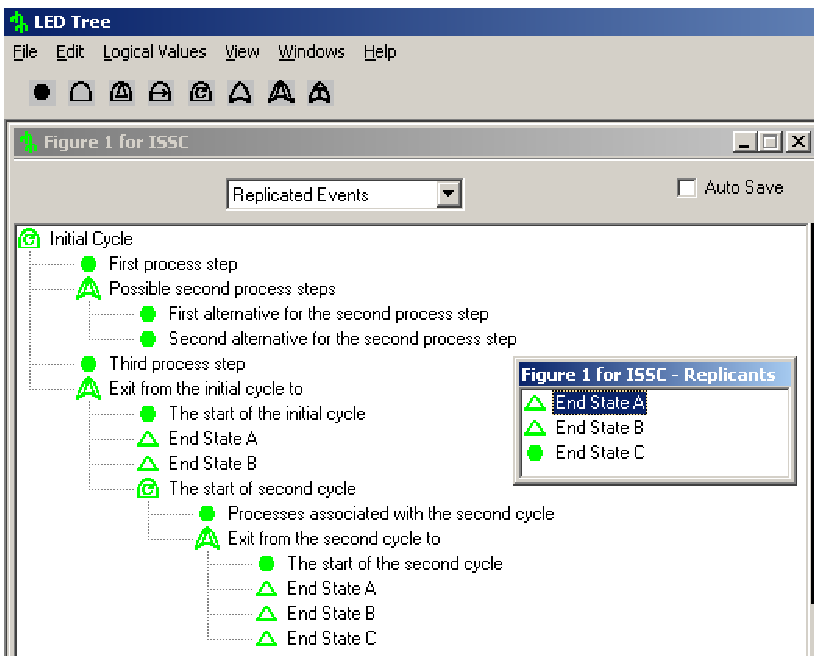

Figure 1 – A Simple Resultant Tree

<u>Solution of the Process Tree</u>: A logic model such as the possibility tree of Figure 1 is more than a simple graphic - it is a logical equation that can be solved. The solutions to this equation are paths leading from the top node to the end states. In this case there are 10 unique paths. The existence of alternative paths arises from the exclusive or gates in the tree. One of the solutions is

> Path = {Initial Cycle, First process step, Possible second process steps, First alternative for the second process step, Third process step, Exit from the initial state to, The start of second cycle, Processes associated with the second cycle, Exit from the second cycle to, End State C}. (1)

We see that this defines an exact sequence leading from the top node to one of our notional end states.

Possibility Tree as a Digraph: Readers familiar with graph theory will have noticed that the logic model described by Figure 1 is not actually a tree.* The paths through this model describe instead a general cyclic digraph. Figure 2 shows this digraph. It is homologous to the logic of Figure 1. In this case we see one source node (*Initial Cycle*) and three sink nodes that correspond to the three end states discussed above. The arcs corresponding to the completion of the cycles are also shown. Each representation associated with the underlying logic here – the possibility tree (figure 1), the alternative paths (eq. 1) and the digraph (figure 2) – provides us with a different view of the problem. The tree provides a compact representation of the logic and the tool to develop complex logic deductively. The paths allow us to examine each unique alternative individually. In LED TREE these paths can be expressed in a linguistic form that facilitates understanding the relationships between the individual elements of the path. Finally the digraph provides a representation that is convenient to examine visually and can be used to help define sets of numerical equations and their interrelationships. We will examine each of these representations next for the cook-off problem.

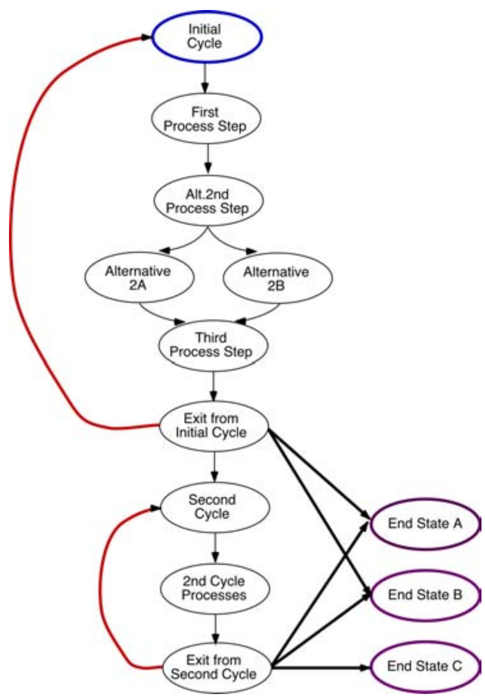

Figure 2 – Digraph Representation for Simple Resultant Tree of Figure 1

A Possibility Tree for Cook-off

The starting point for the development of the cook-off possibility tree for PBX 9501 was a review of the available published literature and an initial series of discussions with HE subject matter experts. An important objective in constructing the tree is to represent in a concise logical form as much of the knowledge base as possible. We constructed an initial tree and then reviewed it with

* This terminology is used for historical reasons.

the experts and made changes as necessary. Additional revisions have been made as research – experimental, theoretical and computational, has continued over the last several years.

During the initial knowledge assessment the decision was made to represent cook-off with a resultant possibility tree. This decision was made based upon the capabilities of the tree software available at the time and the observation that this formulation allowed for the easiest expert elicitation. The initial state in the tree therefore is one where the HE in some thermal environment where heating can occur. The end states in the tree would be those that the HE could reach after the end of cook-off event. These HEVR related end states are actually combined states that describe the degree of HE consumption and the damage resulting from cook-off. The cook-off possibility tree is extremely complicated and it is impossible to describe more than the basic tree structure and then focus on one or two portions of the tree that illustrative an important point. Figure 3 shows an overview of the tree. The open diamonds represent parts of the tree, some quite large, that have been contracted. A gate with a box around the icon is an instance of a replicant and an open triangle indicates a contracted instance of a replicant. There are a large number of replicants, many of which contain in turn other replicants. The presence of these nested replicant structures is indicative of a complex tree.

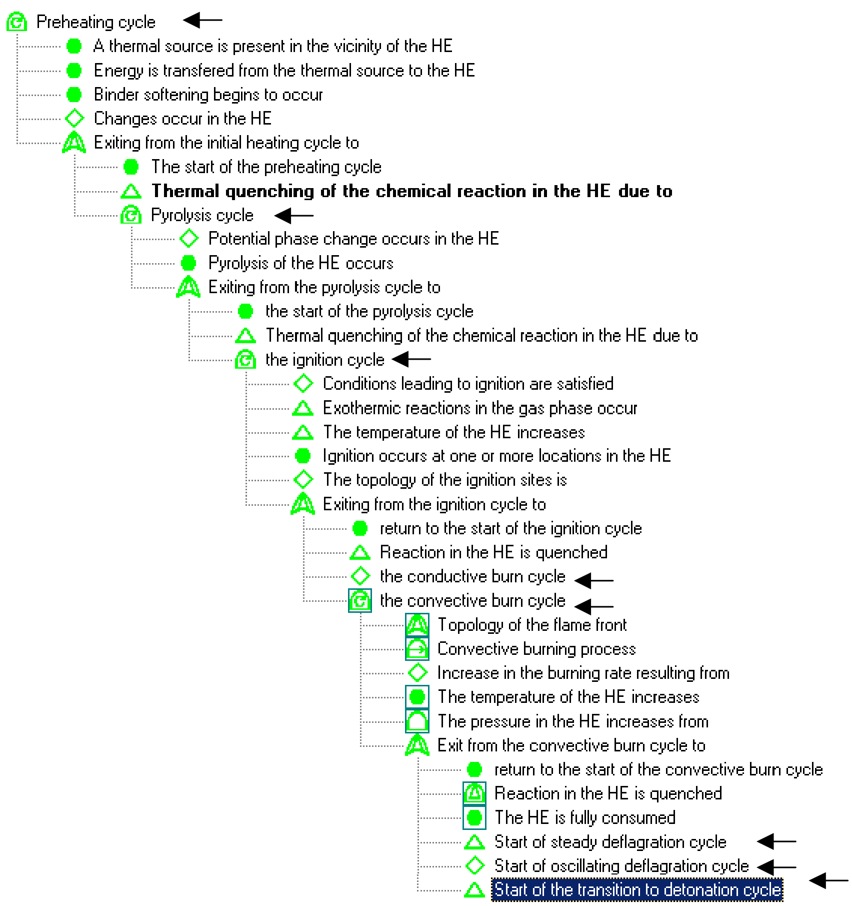

Figure 3 – Overview of Possibility Tree for PBX 9501 Cook-off

Preheating Cycle: The overall structure of this tree is similar to that of Figure 1 with a series of linked process cycles. Each cycle is marked by an arrow. The first cycle at the treetop is *Preheating*. This cycle describes in short form the heat transfer process from the thermal source to the HE and outlines the changes in the HE that result. The changes in the HE may be significant and serve to point out the issue that numerical models will require information about the physical properties of the HE as a function of heating history. The next exit from this cycle is thermal quenching. The rest of this sequence is not shown. The ultimate end states are local decomposition or combustion quenching and possibly local relief of a confined system. The exit leading toward HEVR is the pyrolysis cycle.

Pyrolysis: The next cycle along the path to an HEVR is the pyrolysis cycle. In this cycle chemical changes are occurring in the HE. In PBX 9501 a phase change from β to δ phase HMX is observed during this cycle. The associated change in volume leads to the introduction of cracks into the HE. As discussed below the generation of cracks may be important for post-ignition behavior.

Ignition: The exact definition of the onset of ignition varied among the experts. For the purposes of discussion here we consider it to be associated with the appearance of a flame. An important feature of the ignition is that exothermic reactions are observed to occur in the gas phase. We consider the possibility that ignition may occur at more than one location in the HE and that the topology of these ignition sites may vary.

Burn Cycles: Assuming that the rate of energy generation continues to grow, the ignition cycle concludes with the appearance of conductive or convective burning. That is, there is a distinct reaction wave moving within the HE. We consider that convective burning may occur directly or be an exit from the conductive burning cycle. On the paths to HEVR, the convective burn cycle exits to the steady or unstable deflagration cycles* or to the transition to detonation (TTD) cycle.

Transition to Detonation and Detonation: Figure 4 continues the overview of the possibility tree. The key element here is the generation of a reaction driven pressure wave that is necessary for the deflagration to detonation transition (DDT). Two possible transitions are contemplated – the classic DDT (ref. 2) or a more complex transition associated with plug flow (ref. 4). If the transition occurs then the detonation wave may be stable, over- or under-driven and transitions from these latter two to the former are possible. In all three cases the most interesting result is that a violent disassembly occurs with most of the HE consumed.

HEVR Paths and Digraphs for Cookoff

There are approximately one thousand paths in this tree. Although the details of individual paths and the relationship of sets of paths are an important result of the possibility tree solution, they are beyond the scope of this paper. The digraph representation of the tree is more immediately accessible. Figure 5 shows a simplified digraph where many of the details of Figures 3 and 4 have been subsumed by contractions of subtree developments. Although this digraph was created off-line for inclusion in this paper, a module of LED TOOLS is available to draw digraphs from the path solution and influence diagrams from the possibility tree directly. In this view the details of the individual cycles are replaced by a single arc and the relationship among the cycles and the final states is emphasized.

* We follow the convention that a deflagration wave is a convective flame front moving at the local acoustic velocity. Both the stable and oscillating deflagration cycles have an exit to the transition to detonation cycle.

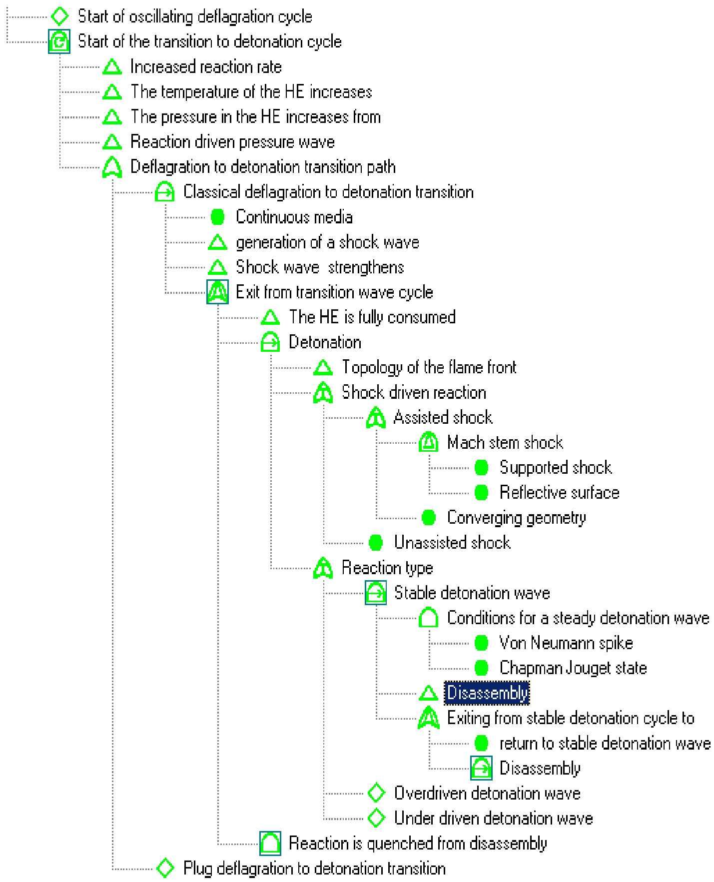

Figure 4 – Overview of Possibility Tree for PBX 9501 Cook-off (cont.)

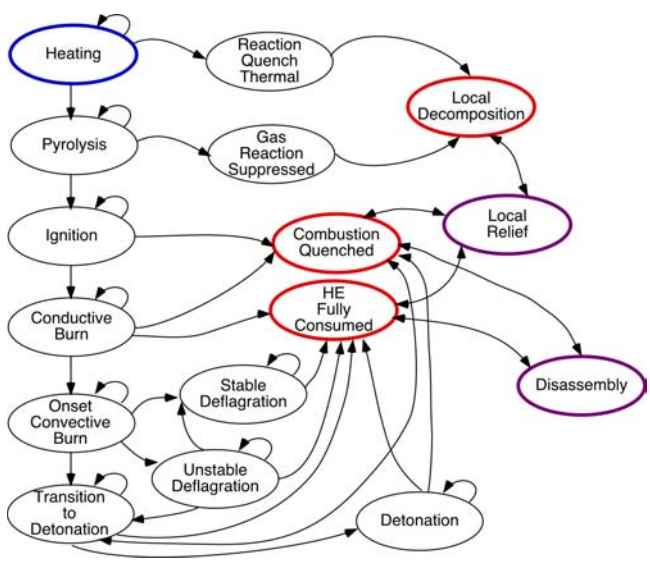

Figure 5 – Simplified Digraph for Representation of the Cook-off Process

Discussion of Results

The hierarchical structure of the possibility tree makes it possible to describe in great detail aspects of the phenomenology where the interrelationships among the processes at work are complex and therefore where many sub-paths may exist. One aspect of cook-off where this situation arises is the phenomenon of reaction spreading. Figure 6 shows the associated digraph for this segment of the possibility tree. In this case development of the tree lead to development of a numerical model that models the motion of reactive gases in the HE using a Darcy law approximation. Calculations with this model showed that gas phase transport in thermally damaged HE is an important process in predicting time and location of ignition and therefore in reaction violence.

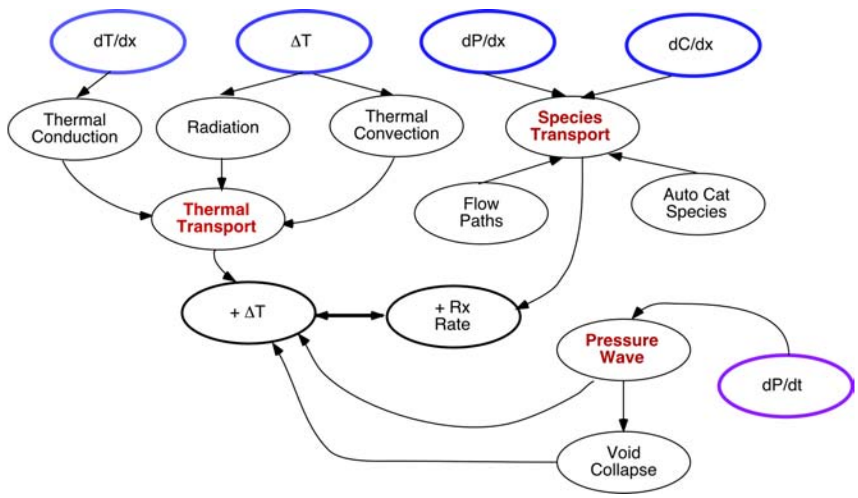

Figure 6 –Digraph for Reaction Spreading Processes

Conclusions

Possibility trees provide a powerful tool for developing models of complex physical processes. The key to this capability is the use of deductive logic to describe the details of a process and the interrelationships between sub-processes. The LED TOOLS software facilitates the development of the logic structure by providing a graphical user interface that encourages problem formulation using natural language descriptions. This encourages subject matter experts to interact and provides a structure to integrate the available knowledge base.

We have applied these methods to the problem of cook-off in PBXs. The possibility tree is a comprehensive logical representation of the phenomenological paths from the heating of the HE to the final states of the system. This logic can also be represented as a digraph. The use of trees and digraphs to visualize the relationships between physical processes is a valuable tool in the development of physical models.

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